

substance: Ta₂O₅

property: crystal structure and related parameters of H-Ta₂O₅

The Ta–O phase diagram appears to show only one thermodynamically stable phase, Ta₂O₅.

Ta₂O₅ exists in two forms, L- or β-Ta₂O₅, stable below 1320°C, and H- or α-Ta₂O₅, which is the stable form at high temperature. Kinetics of transformation are slow and H-Ta₂O₅ is therefore the form available as crystals at 300 K and for which the data reported below pertain. H-Ta₂O₅ melts at 1872°C [56R].

H-Ta₂O₅

crystal structure: monoclinic, space group C2, *Z* = 6, retains the distorted bipyramids of the L-form [71S], (010) projection of the structure: Fig. 1.

lattice parameters

<i>a</i>	35.966 Å	71S
<i>b</i>	3.810 Å	
<i>c</i>	3.810 Å	
<i>β</i>	96°7'	

For interatomic distances, see [71S].

Other structures have been reported for Ta₂O₅. An orthorhombic form has been found in films grown below 700°C with *a* = 5.47 Å, *b* = 7.65 Å, *c* = 26.10 Å. Its structure has been likened to the perovskite tantalates [72K].

density

<i>d</i>	8.2 g cm ⁻³	83H
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References:

- 56R Reisman, A., Holtzberg, F., Berkenblit, M., Berry, M.: J. Am. Chem. Soc. 78 (1956) 4514.
71S Stephenson, N. C., Roth, R. S.: J. Solid State Chem. 3 (1971) 145.
72K Khikova, V. I., Klechkovskaya, V. V., Pinsker, Z. G.: Kristallografiya 17 (1972) 506.
83H Handbook of Chemistry and Physics, Weast, R. C., (ed.), 64th edition 1983, CRC Press, Inc.

Fig. 1.

H-Ta₂O₅. A (010) projection of the structure. Heavily shaded polyhedra are located at $y = 1/2$ and the remainder are at $y = 0$ [71S].

